

## **WG2: Leeds University – 23/1/2014**

### *Present:*

Stuart McNicholas, Ronan Keegan, Arwen Pearson, Ivo Tews, Liz Potterton, Charles Ballard, Eugene Krissinel, Sidhu Khushwant, Andy Purkiss, Arnaud Basle, Jose Trincao

*Chair:* Arwen Pearson

*Minutes:* Ronan Keegan

### *Agenda:*

- Core Group Report
- Role of WG2?
- Debrief on SW 2014
- Plan for SW 2015
- CCP4i2 demonstration

Approved previous minutes

### *Matters to add to agenda:*

CCP4Forge

### *Chairs Report:*

SW 2014 – CB to report

Thanks to Jon & Ivo

## **EK: Report on Core Group Activities (See presentation for full details)**

### *Modernisation:*

- Software repositories (CB, VU, MW)
- New build system (MW)
- Nightly build (CB, VU, MW)
- New release mechanism (VU, CB, RK, AL & EK)

SMcN & LP are using elements of the above for their developments

EK displayed the CCP4 Modernisation diagram:

Test framework and Autotests are nearly done, everything else is pretty much complete

### *Software maintenance:*

- Current Activities:
- Bug fixes
- Interface developments and modernisation (CB, RK, AL)
- Preparations to the PDB format change (EK)
- Tests (VU, CB)

### *Releases and Updates:*

Current activities and highlights

- CCP4 6.4.0 released in October 2013
- Update Series (AL, EK)
- Platform break-down: Windows is biggest single download but Linux and Mac may be centralised installations and therefore have more users. AP pointed out that in Universities it

- is possible that a lot of educational machines are Windows machines.
- Geographical breakdown (see EK presentation for full details):
  - US – 21%
  - China – 12%
  - Next: Japan, UK, etc...

APu: What about getting access to where CCP4 is being run rather than downloaded to? Maybe possible but implementing it and getting user and STFC consent could be too problematic.

#### *Software developments:*

- DIALS (David) – new diffraction image processing
- AMPLE (Ronan) – Solved novel structures
- PISA (Eugene) – scoring interfaces,
- Other – Ctruncate, ViewHKL, other components
- multiple structure alignment in SSM (EK)
- BALBES – server now improved and stable
- MrBUMP – server to come

Updates to come (possibly next release) – New Phaser, iMosflm (Multiple Lattice), BLEND, AMPLE dependencies, Crank2, Tassos Software – PDBRedo

SK: There can be problems with updates when using a central Mac server – mount point is different (/Volumes) on client machines. Some updates hard code into program the path and clients get messed up. ARP/wARP is one example.

**ACTION:** SK to send Charles details next time it happens

**ACTION** EK: to check that updates are on relative paths – should be this way

#### *Outreach Activities:*

##### 2013 Workshops:

- CeBEM/CCP4 Workshop, Montevideo, April 2013
- APS/CCP4 School, Chicago, June 2013
- CCP4/OIST School, Okinawa, Japan, November 2013

##### Upcoming Workshops:

- Sao Carlos, Brazil in April 2014
- APS School, Chicago in June 2014
- Japan (possible), late 2014
- Diamond (possible), December 2014

##### Other Workshops:

- EMBL-Hamburg, April 2013 (CB and David Waterman)
- Oulu – September 2013 (Andrey Lebedev)

##### Conferences:

- ACA, Hawaii, July 2013
- ECM, Warwick, August 2013
- AsCA, Hong Kong, December 2013

LP: Asked to be kept up-to-date on conferences: ACA 2014 (Albuquerque, May), iUCR 2014

WG2: Leeds University Jan 23<sup>rd</sup> 2014

(Montreal, August)

Other outreach activities:

- CCP4 now taking part in Diamond Bag training

## **AP: Role of CCP4 WG2**

CB: How can we get more people to come to meetings?

IT: Who uses the software and target them individually – contact them at labs or at Diamond

Make it clear that CCP4 pays for travel

AB: He is here because of discussions with MN at Newcastle

Mention at CCP4 Study Weekend

Coal face people rather than group leaders

AB: Re-brand WG2?? No

How big is the email list? – Large number registered

Used to be a developers forum – not so many developers any more

It was felt that WG2 should complement the developers meeting by being a forum for communication between the users and the developers.

IT: What can be offered by WG2 to potential attendees?

- Developers to speak about new developments
- Groups of Universities could provide regional representatives

IT: Should the meeting move around to catch different areas? Should we have it more often e.g. 3/4 times a year? It was felt that 3 a year may be the best scenario, one in London and 2 others in the regions - January, early summer and September or October? The autumn meeting would give SW organisers the chance to give feedback on selected speakers.

CB: London meeting is biggest – when should it be? AP: It should be the summer meeting

It was suggested that there be a developers get-together probably in Cambridge? This could be done this summer for a change. In the MRC with Garib or Andrea as suggested organisers.

AP: Somebody from EBI/PDB could come too.

Targeted invites could be sent to all groups

RK: What date for this meeting: June – provisionally Wednesday 11th June

**ACTION:** CB to send WG2 mailing list to Ivo and Arwen

**ACTION:** IT/AP to contact Cambridge groups and arrange June meeting

IT: What is the remit of this group? Can we have it in writing –

**ACTION** IT to draft something and send it round for consideration

*Lunch..*

## **CB: Debrief on SW 2014:**

- There were some minor complaints about accommodation, food and lunch time queues.
- Numbers: 356 attended out of 372 who registered
- Country breakdown: 2/3=UK, next=US (30)
- 145 Students
- More bursaries were given out this year

*IT: Feedback from attendees:*

- Students: Structural Biology students liked it, MX students wanted more crystallography
- Overall – the meeting was well liked and appreciated. Some had been sceptical but said it turned out to be very useful. Others said that it shouldn't be like this every year but was very useful
- IT: Should it be done like this again? Yes – but not too far out of scope of CCP4 and only once in every few years.
- AP: Electron Microscopy session was deemed the favourite from feedback she received.
- Drug design session was only of interest to people actually working in that area
- Lunchtime bytes were well appreciated (Nick Keep)
- Different topics for different sessions: How well did that work? Overall good?
- There was a question about where do postdocs get their money for SW? Costs add up quickly. It was felt that Postdocs should have grant support for meetings like this.

**ACTION CB:** Find out how many viewers watched on the live stream

*What was good experience for future meetings:*

- AP: There is a need for a tutorial session at the start of each topic session.
- IT: Chairs in contact with speakers – worked very well. Helps chair to not replicate contents of speakers
- IT: 2 deadlines were set: 5 and 16th of September. Talks stored on disk and chairs could review them. There was 50% compliance. Good for chairs to target their introduction – very useful!!

**ACTION** to implement this in future

**ACTION IT** to tutor next organisers in doing this

- AP: There should be a split into methods and applications talks
- IT: How was the quality of discussions? Same as usual, usual suspects asked questions. Should we have lively discussions or not? Yes!! More diligent timing of talks would help this.

**SW 2015:**

Possible locations: Royal Holloway, Nottingham, Warwick on short list so far. Final decision very soon.

Aiming to stage it in the second week of January (7/8/9)

*Topics for 2015:*

- Experimental Phasing – old methods, new sources (from last year's minutes)
- DIALS and processing data, new sources and methods
- AP (from Harry Powell): Meeting should be educational and periodical. It doesn't matter if there isn't anything new. How will this affect the written proceedings? We are allowed review articles. Not a problem.
- IT: What Topics? Pipelines & Workflows, CCP4 rollouts? Diamond stuff, EM beamlines, XFEL, crystallisation? Keep in mind the link to other CCP's. Phasing membrane proteins, novel phasing.

- AP: Experimental Phasing: multicroystals, SIRAS, MIRAS, MR-SAD, Soaks, and stuff about new sources - Diamond and others, Density modification

Organisers: TBD (**ACTION** IT and AP)

## **LP: CCP4I2 demonstration:**

Should there be an alpha-test soon?

Should bug tacker be used for alpha-testers? Possibly

AB: Looks nice on mac but not so good on Linux machines – related to icons from system. Difficult to harmonize.

Who should write the wrappers? – Developers of software

How to start writing wrappers?

1. Go to developers intro html page (in gui)
  1. How to get to CCPForge
  2. Defined types
2. Copy template
3. Write 3 different methods
  1. ProcessInputFiles
  2. ProcessOutputFiles
  3. MakeCommandAndScript

Other new features:

- Can import and export projects
- Can import XIA2 runs from DLS
- Coot interaction
- Coot function calls

CCP4i XIA2 interface requests: **ACTION** RK.

- Resolution
- Slice out images
- Discontinuity scaling

ACTION all to test gui2

## **Other business:**

- MG: New release at Christmas
- SK: Why does CCP4 not use CCPForge? CB: CCP4 has its own forge:
  - *fg.oisin.rc-harwell.ac.uk*
- AP officially handed over chair position to IT. Everybody congratulated IT on his new role and AP for all her efforts.

## **Next Meeting:**

Provisionally Cambridge (June 11<sup>th</sup> 2014)